Preview of Award 0901514 - Final Project Report

Cover

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PD/PI Name:	Jean Bellissard, Principal Investigator
Submitting Official (if other than PD\PI):	Jean Bellissard Principal Investigator
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Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	Jean Bellissard

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Accomplishments

*** What are the major goals of the project?**

1)- Atomic Diffusion: Description of atomic diffusion in aperiodic solids with *Finite Local Complexity* (FLC)through a Laplace-Beltrami operator on the Transversal of the solid. The Pearson Laplacian was a potential candidate. But finding showed that this program requires a better description of the corresponding Geometry

1a)-Are there metrics on the transversal for which it becomes bi-Lipshitz embeddable into a finite dimensional Euclidean Space?

1b)-Can one extend the Pearson Laplacian to the C*-algebra of the groupoid of the transversal? This question also required a better description of this groupoid.

2)-Non-finite Local Complexity: Is it possible to extend the previous study to solid without finite local complexity ? This question requires to be refined, namely which system can be described in a way similar to FLC, through an inverse limit

2a)-In the proposal the concept of semifinal complexity was introduced.

2b)-It was proposed to construct the Cech cohomology of the Hull through a spectral sequence

3)-Dissipative Transport: The last goal of the proposal was to investigate the problem of dissipative transport in solids, in particular the most challenging problem for a mathematician, namely the Mott hopping transport.

*** What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?**

Major Activities: **1)- Atomic Diffusion:**

1a)- the *embeddability problem* has been solved completely recently in a paper with A. Julien. The initial tool used to answer this question, namely the concept of Michon graph, providing a combinatorial description of the transversal, has been recently supplemented by using the concept of Assouad dimension of metric spaces. Embeddability implies that the Assouad dimension is finite. The converse is almost true, namely instead of bi-Lipshitz embeddability, finite Assouad dimension implies Hölder embedability for all Hölder exponent <1. In the ultrametric case, finite Assouad dimension is equivalent to bi-Lipshitz embeddability. In the work with A. Julien, it was showed (i) how to translate the Assouad language in terms of the Michon tree, (ii) which tiling spaces are embeddable, giving many classes of examples and counter-examples.

1b)- extending the Pearson Laplacian, was investigated in a paper with M. Marcolli and K. Reihani. This paper has not been published though. However, *it was proved that there is an obstruction* to this extension to be available. This *obstruction* can be described as follows: having a metric structure on the transversal leads to a spectral triple (I. Palmer PhD Thesis). Extending it to the groupoid is possible if and only if the translation acts by isometries. A result by I. Putnam shows that the metrics defining the tiling space topology are always leading to a translation group action that is hyperbolic, thus certainly not isometric. To get out of this major obstruction, an idea was proposed: use the *metric bundle* approach of Connes and Moscovici. This aspect was investigated in some specific cases in the paper cited above. However the general theory is still to be made. The PI has started a collaboration with F. Latrémolière (U. Denver, CO) who proposed to use the approach proposed by M. Rieffel, because it leads to a good definition of the metric bundle in the noncommutative case. This work is under way

2)-Non-finite Local Complexity: the PI has not yet published any paper yet on this issue but has written a *100-page document* containing many new results. In particular he met with several experts of bulk metallic glasses during two visits to the Material Science Institute (Tohoku U., Sendai, Japan) in February 2012 and then in June 2012 and he realized that his work on non-FLC could be used efficiently to give an atomic scale description of metallic glasses. Among the experts was T. Egami, who is the Director of the Joint Institute of Neutron Sciences at Oak Ridge, TN, and started a collaboration with him. Amazingly, Egami told the PI that describing the liquid phase might be a better starting point. Indeed it seems to provide a very simple Statistical Mechanical description of liquid through realizing that the dominant degrees of freedom in liquids are "bonds" that the PI has proposed to call "anankeons", which behave like free independent particle described through their stress tensor. The free anankeon theory is as simple as the usual free perfect gases and gives an explanation for the behavior of the heat capacity and presumably of the viscosity. The main contribution of the PI in these directions are the following

(i) a detailed description of the configuration space through using Delone graphs, analyzing the most likely configurations. The concept of *Delaunay (Delone) triangulation* coincides with the concept of *Delone graphs*.

(ii) realizing that the bond motion can be described through what is known in Geometry under the name of "*Pachner Moves*" (collaboration with T. Kondo and Nogawa, Sendai, Japan)

(iii) The set of Pachner moves leads to the concept of "*contiguity graphs*", describing in a combinatorial way which changes in configurations is most likely to occur.

(iv) The bond dynamics is proposed to be described through a *Markov process* *on the contiguity graph*.

This scheme seems to fit in many details the numerical simulations made by Egami and coll. It seems to be the right direction to follow. The main difficulty though is to describe accurately the interaction between anankeons and phonons. In the liquid phase, the non acoustic phonons are damped too quickly due to the bond dynamics and can be neglected. At low temperature, the bonds are frozen and cannot move much, leading to restoration of phonons as the main degrees of freedom. The glass transition involves in a crucial way the description of the interaction between these two families of degrees of freedom. This can only be made through a thorough description of bond deformations liable to lead to an atomic scale description of the theory of elasticity.

One important ingredient in this approach is the shear transformation zone theory (STZ) proposed by Falk and J. Langer in 1998, which gives macroscopic equations liable to go beyond the elasticity theory. A very good description of the plasticity region has been obtained by the Langer group in terms of nonlinear PDE, called here the STZ equations, in a way similar to the Navier-Stokes equations, extending the usual theory of elasticity. An amazing work by Chris Rycroft (UC Berkeley and Harvard) showing a numerical simulation of irreversible plastic deformation using the STZ equations.

3)-Dissipative Transport: a paper has been published in collaboration with G. Androulakis and C. Sadel in which the description of a noncommutative Markov dynamics has been proposed to describe the electronic motion in a semiconductor at very low temperature (variable range hopping transport). This Markov process describes the equilibrium dynamics as well as the non equilibrium one.

However the PI has not yet succeeded in making the bridge with the Mott theory leading to a prediction for the conductivity. This is why the PI is pursuing the collaboration with C. Sadel. A thorough study of the physics literature of the early seventies on this topics are giving hints about which strategy to use to give a rigorous proof of the Mott prediction.

Specific Objectives: See above

Significant Results:

1)- Embeddability: An explicit necessary and sufficient condition for embeddability of the transversal for tilings or atomic distributions with FLC

2)- Extension to the Tiling C*-algebra: An obstacle to extend the noncommutative Riemmanian structure of the transversal to the tiling C*-algebra has been discovered. A solution to go around this exists in commutative geometry, but the noncommutative analog does not exist yet

3)-A quantum model for variable range hopping transport in Semiconductors at Low Temperature.

4)-Serious progress in describing complex aperiodic solids.

Key outcomes or Other achievements:

5)-Scattering theory for Bloch electrons in a periodic lattice scattered by a local impurity in dimension *d=3* and above. Collaboration with H. Schulz-Baldes. This work proves the Levinson Theorem in this case and is seen as an Index Theorem. This result requires to go way beyond the results accessible in the literature, in that the scattering operator is comoputed globally over the entire spectrum.

6)-Noncommutative Chern Numbers for 3D-Topological Insulators with disorder. Collaboration with E. Prodan and B. Leung. An extension of the work on the Quantum Hall Effect (Bellissard, Van Elst, Schulz-Baldes 1994) is leading to a formula for the second Chern class used to describe the topological part of the magneto-electric response function (Wang 2006). This formula, initially proved for periodic crystals is valid in presence of disorder.

*** What opportunities for training and professional development has the project provided?**

Two **REU undergraduate students** were trained during ther Summer 2010.

(i) *Jonathan Paprock*i: work on the proportion of phason flips in the two-dimensional octagonla lattice.

(ii) *Greg Douthit*: work on the spectrum of one-dimensional hamiltonians on an aperiodic FLC tiling.

One **PhD Studen**t was trained between 2009 and 2013

Robert Parada: work on a model of Statistical Mechanics liable to describe the solidification of an aperiodic Fibonacci chain.

*** How have the results been disseminated to communities of interest?**

5 invited minicourses

12 invited talks in Conferences, Workshops, Colloquium and Seminars. See

http://people.math.gatech.edu/~jeanbel/talksjbE.html

Products

Journals

E. Prodan, B. Leung, J. Bellissard (2013). The non-commutative n-th Chern number. *Journal of Physics A*. 46 (48), 485202.

Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: doi:10.1088/1751-8113/46/48/485202

J. Bellissard, A. Julien (2013). Bi-Lipshitz Embedding of Ultrametric Cantor Sets into Euclidean Spaces. *Ergodic Theory and Dynamical Systems*. .

Status = UNDER_REVIEW; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

J. Bellissard, H. Schulz-Baldes (2012). Scattering theory for lattice operators in dimension d≥3. *Review in Mathematical Physcs*. 24 (8), 1250020.

Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: DOI: 10.1142/S0129055X12500201

Androulakis G., Bellissard J., Sadel C. (2012). Dissipative dynamics in semiconductors at low temperature. *Journal of Statistical Physics*. 147 (2), 448.

Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; ISSN: ISSN: 0022-4715

Books

Book Chapters

Thesis/Dissertations

Conference Papers and Presentations

Other Publications

Technologies or Techniques
Nothing to report.

Patents
Nothing to report.

Inventions
Nothing to report.

Licenses
Nothing to report.

Websites

Title: Jean Bellissard

URL: http://people.math.gatech.edu/~jeanbel/

Description: All information about the PI, biography, Research, publications and talks can be downloaded in pdf format, teaching activities and web site of each courses.

Other Products
Nothing to report.

Participants

Research Experience for Undergraduates (REU) funding

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Robert Parada	Graduate Student (research assistant)	12
Jean Vincent Bellissard	PD/PI	12

What other organizations have been involved as partners?
Nothing to report.

Have other collaborators or contacts been involved? N

Impacts

What is the impact on the development of the principal discipline(s) of the project?

The ultimate goal of the program is to develop a mathematical theory liable to describe the physical properties of all aperiodic solids and perhaps liquids as well. Are involved the electronic properties, the electronic transport, the diffraction and propagation of various waves degrees of freedom (phonons, spinon), the description of the structure of the solid, of the atomic movement, the passage from a microscopic to a macroscopic description of mechanical properties (elasticity, plasticity, fractures, viscosity for liquids).

The materials involved can be semiconductors at low temperature (disordered systems), crystals in magnetic field, aperiodic solids with long range order (such as quasicrystals), bulk metallic glasses and their liquid phase. The mathematical framework offered covers all these situation already

The Mathematical Approach uses the tools developped for Noncommutative Geometry, including K-theory and cyclic cohomology (for topological invariants), Topology and topological Groupoids, combinatorial description through graph theory, CW-complex and triangulations, metric Geometry, Markov processes (to describe the dynamics).

This program is ambitious in that it intend to account in a coherent way of multiple contributions made for each categories of materials, independently, with particular modelings.

The PI started this program in 1979 and is now reaching a stage where a compilation of results (review, book) becomes necessary.

What is the impact on other disciplines?

The most spectacular finding in this program were the **Gap Labeling Theorems**, and the theory of the **Integer Quantum Hall Effect** from first principles, including the presence of disorder and of dissipation. More recently this formalism has been used to show the robustness of topological invariant in **topological insulator**s with respect to the presence of disorder. The work of Emil Prodan (Yeshiva University) shows that implementing this formalism to perform numerical calculations leads to much more **efficients algorithms**.

The hope of the PI is to have a contribution in the mechanical properties of the bulk metallic glasses. The general formalism developped earlier, gives a precise description of the structure, and is compatible with the cluster theory developped by Egami and Miracle, as well as with the bond theory of Egami. The search of a microscopic description of the dynamics through the "bond" and "phonon" degrees of freedom is the next step.

What is the impact on the development of human resources?

The present project has provided an opportunity to train REU students (jonathan Paprocki, Greg Douhtit) and PhD students (Robert Parada)

What is the impact on physical resources that form infrastructure?
Nothing to report.

What is the impact on institutional resources that form infrastructure?
Nothing to report.

What is the impact on information resources that form infrastructure?
Nothing to report.

What is the impact on technology transfer?
Nothing to report.

What is the impact on society beyond science and technology?
Nothing to report.

Changes

Changes in approach and reason for change

The part of the project concerning **Non-finite Local Complexity** has been changed substantially after the PI met with the expert of *bulk metallic glasses* in Sendai in February 2012. The formalism used today is entirely different from the approached summarized in the original proposal. At the same time, it is more realistic and closer to experimental results.

Actual or Anticipated problems or delays and actions or plans to resolve them
Nothing to report.

Changes that have a significant impact on expenditures
Nothing to report.

Significant changes in use or care of human subjects
Nothing to report.

Significant changes in use or care of vertebrate animals
Nothing to report.

Significant changes in use or care of biohazards
Nothing to report.